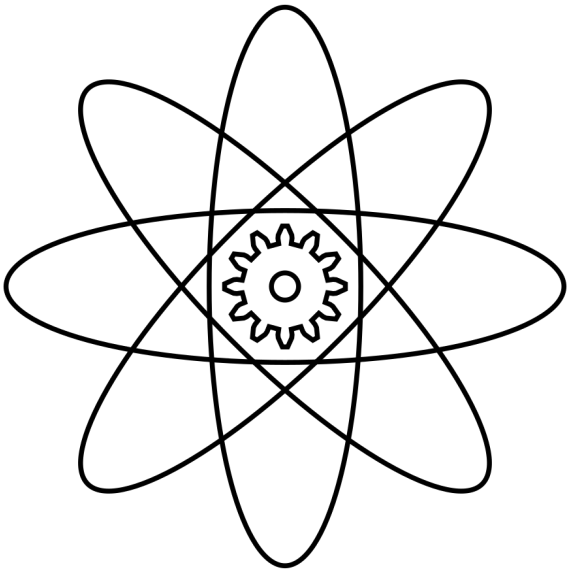

Machine Learning for Quantum Matter

Aug 26-28 2019; Nordita, Stockholm, Sweden

NORDITA

KTH VETENSKAP OCH KONST

Stockholm University

Scope of the Workshop

Over the past decades we have witnessed an enormous increase of computational power and a rapid development of experimental techniques. Both developments, together with the great advancements of data storage capacities have initiated the application of methods taken from computer and data science into the research of functional quantum materials and quantum many-body physics.

This conference aims to bring together internationally leading scientists working on the intersection between condensed matter physics and computer science. It is intended to exchange knowledge about the current state-of-the-art machine learning tools applied to condensed matter physics. The scope covers topics such as quantum simulation and quantum computation, quantum materials and materials design, exploring the chemical space, machine learning for magnetism, as well as methods and algorithms.

Funding sources

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Timetable

Monday, Aug 26th

09:30 - 09:45	Introduction (A. Balatsky)
	Quantum Simulations and Quantum Computation (chair A. Balatsky)
09:45 - 10:45	*Jacob Biamonte* - Quantum Machine Learning for Quantum Simulation
10:45 - 11:00	Coffee break
11:00 - 12:00	*Mats Granath* - Quantum error correction for the toric code using deep reinforcement learning
12:00 - 14:00	Lunch break
	Quantum Materials and Materials Design (chair J. Bardarson)
14:00 - 15:00	*Matthias Geilhufe* - Organic Quantum Matter and the Organic Materials Database
15:00 - 16:00	*Valentin Stanev* - Machine learning modeling of superconducting critical temperature
16:00 - 16:30	Coffee break
16:30 - 17:00	*Oleksandr Balabanov* - Unsupervised detection of topological quantum state equivalences
17:00 - 17:30	*Ali Mazhar* - Deriving descriptors from fundamental physical models for targeted material property prediction using machine learning
18:30 - 21:00	**Reception at Alba Nova**

Tuesday, Aug 27th

	Exploring the chemical space (chair B. Olsthoorn)
09:00 - 10:00	*Alexandre Tkachenko* - Towards Universal Machine-Learning/Physics Model of Molecular Properties in Chemical Space

10:00 - 10:15	Coffee break
10:15 - 11:15	*Anatole von Lilienfeld* - Navigating chemical space with quantum machine learning
11:15 - 12:15	*Artem Oganov - Artificial intelligence methods for discovering novel materials and exotic compounds*
12:00 - 14:00	Lunch break
	Magnetism (chair M. Geilhufe)
14:00 - 15:00	*Rio Tamura* - Effective model estimation for magnetic materials by machine learning
15:00 - 16:00	*Johan Hellsvik* - spin wave excitations of magnetic metal organic materials
16:00 - 16:30	Coffee break
16:30 - 17:30	*Johan Mentink* - New horizons for the fastest, densest and least dissipative brain-inspired computing

Wednesday, Aug 28th

	Methods and algorithms (chair M. Geilhufe)
09:00 - 10:00	*Kristof Schütt* - SchNet - an interpretable atomistic neural network
10:00 - 10:15	Coffee break
10:15 - 11:15	*Tess Smidt* - Euclidean Neural Networks for Emulating Ab Initio Calculations and Generating Atomic Geometries
11:15 - 11:45	*Caroline Brembilla* - Phylogenetic operads in machine learning
11:45 - 12:15	*Joana Olivia* - Microsoft's Azure ML and AI modeling portfolio
12:00 - 14:00	Lunch break
	Outline (chair J. Bardarson)
14:00 - 15:00	*Alexander Balatsky* - Dirac Materials and Informatics
15:00 - 15:30	*Yi Luo* - Determining spectrum-structure relation with machine learning techniques
15:30 - 16:30	Coffee and round table discussion

Abstracts

Quantum Machine Learning for Quantum Simulation

Jacob Biamonte, Skolkovo Institute of Science and Technology

"Simulators" are an emerging class of computational devices which aim to augment traditional computer programming by accelerating certain subroutines. Many computer algorithms—particularly in machine learning—were inspired by, or are closely related to, naturally occurring physical processes. The simulator replaces computer code which mimics a physical process with a physical process itself. Typically physical processes of interest include those which minimize a systems energy (which can be utilized to solve optimization problems) as well as making multiple measurements of a system which can simulate Gibbs sampling. In our effort to merge quantum simulators with machine learning, we tell a story that is as pessimistic as it is optimistic. We recall several recent new discoveries that help shed light on what noisy quantum processors will be cable of, including some insights towards what classes of problems they can and cannot solve.

Quantum error correction for the toric code using deep reinforcement learning

Mats Granath, University of Gothenburg

Surface codes that provide topological protection for logical qubits are believed to be one of the most promising avenues towards robust quantum computing. An important ingredient in the successful operation of a surface code qubit is the decoder protocol for quantum error correction, based on the incomplete diagnostics (the syndrome) of the noisy state of the system. In this talk we present work on Kiteav's toric code, where we develop an AI-based decoding agent that uses deep reinforcement learning. The trained agent suggests error correcting Pauli operations on physical qubits based on the action-value Q-function, which is represented by a deep convolutional neural network. For moderate code lengths we find that the AI-agent outperforms the standard decoding algorithm, showing the promise of using machine learning for this task.

P. Andreasson et al. arXiv:1811.12338 2018;

M. Eliasson et al, in preparation

Organic Quantum Matter and the Organic Materials Database

R. Matthias Geilhufe, Nordita

Quantum matter represents a class of materials where quantum phenomena are dominant over a wide range of energy and length scales, such as superconductors, topological semimetals, or spin- and charge-quantum liquids. Due to their complex crystal structure and strong correlation effects organics have remained a niche in quantum materials research, despite a few prominent exceptions. Recent developments in materials informatics have opened the path towards novel tools for organic quantum materials discovery which I will discuss throughout the talk. My talk presents the development of the organic materials database - OMDB, a freely accessible electronic and magnetic structure database for previously synthesized 3-dimensional organic crystals, available at https://omdb.diracmaterials.org [1]. I will show recent progress in using machine learning algorithms on highly complex organic structures [2] and outline their consequences in future quantum materials discovery.

[1] S. S. Borysov, R. M. Geilhufe, & A. V. Balatsky, PloS one 12.2, e0171501 (2017)

[2] B. Olsthoorn, R. M. Geilhufe, S. S. Borysov, A. V. Balatsky, Adv. Quant. Tech., 1900023, (2019)

Machine learning modeling of superconducting critical temperature

Valentin Stanev, University of Maryland

Machine learning has emerged as a powerful new research tool that can be used to answer scientific questions in unconventional ways. In this talk I will discuss how it can help us address one of the most challenging problems in the study of quantum matter – finding connection between superconductivity – in particular superconducting critical temperature T_c – and chemical/structural properties of materials. I will present several recently developed machine learning methods for modeling the T_c of more than 12,000 known superconductors available via the SuperCon database. These models use coarse-grained predictors based only on the chemical composition of the materials. They demonstrate strong predictive power, with learned predictors offering insights into the mechanisms behind superconductivity in different families. The models can be combined into a single pipeline and employed to search for potential new superconductors. Searching the entire Inorganic Crystallographic Structure Database led to the identification of 35 compounds as candidate high-T_c materials. I will also discuss how machine learning can be used to guide and accelerate the experimental process in a specific superconducting family.

Unsupervised detection of topological quantum state equivalences

Oleksandr Balabanov, University of Gothenburg

I will present an unsupervised computational scheme for detecting topological quantum state equivalences and demonstrate it on simple examples in 1d. The idea is to apply the “learning by confusion” protocol [Nat. Phys. 13, 435-439 (2017)] on datasets of topologically equivalent states produced using unbiased exploration. This exploration, inspired by data augmentation techniques for image recognition, is developed to efficiently survey the relevant topological equivalence classes, enabling one to create the datasets for the neural-network-based classification. The scheme will be explicitly illustrated on concrete examples in 1d where the topological state equivalences and distinctions will be correctly predicted without any prior knowledge of the topological invariants. [O.B. and M. Granath, in preparation]

Deriving descriptors from fundamental physical models for targeted material property prediction using machine learning

Ali Mazhar, Max-Planck-Institute for Microstructure Physics Halle

As ML and AI technologies become more mature, their application to condensed matter physics problems becomes more tractable. However, it is important to identify what problems are the most beneficial to tackle as well as develop fundamental physical models which are able to be integrated into ML models. In particular, prediction of material properties or novel materials with properties which lay in Pasteur's Quadrant are of great interest both from the perspective of fundamental physics as well as technological application. Here we will discuss some of the desired directions of materials AI research, with a particular focus on the spin and anomalous hall effects for device electronics. We will explain the physical model and subsequently derived major descriptor for predicting these properties and briefly discuss how this can be integrated into materials databases and materials AI.

Towards Universal Machine-Learning/Physics Model of Molecular Properties in Chemical Space

Alexandre Tkachenko, University of Luxembourg

"Mindless" learning from data has led to paradigm shifts in a multitude of disciplines. Can machine learning enable similar breakthroughs in “understanding” (quantum) molecules and materials? Here, the two main challenges are: (1) the disproportionately large size of chemical space, even when only counting small organic drug-like candidates, (2) the complex nature of quantum interactions on different length and time scales. Aiming towards a unified machine learning (ML) model of quantum interactions, I will discuss the potential and challenges for using ML techniques in chemistry and physics. ML methods can not only accurately estimate molecular properties of large datasets, but they can also lead to new insights into chemical similarity, aromaticity, reactivity, and molecular dynamics [1]. However, to do so one needs to carefully unify spatial and temporal physical symmetries with purpose-designed ML methods [2,3]. While the potential of machine learning for revealing insights into complex quantum-chemical systems is high, many challenges remain. I will conclude my talk by discussing these challenges.

[1] K.T. Schütt, F. Arbabzadah, S. Chmiela, K.R. Müller, and A. Tkatchenko, Quantum-chemical insights from deep tensor neural networks. Nature Commun. 8, 13890 (2017).

[2] S. Chmiela, A. Tkatchenko, H.E. Sauceda, I. Poltavsky, K.T. Schütt, and K.-R. Müller, Machine Learning of Accurate Energy-Conserving Molecular Force Fields. Science Adv. 3, 1603015 (2017).

[3] S. Chmiela, H. E. Sauceda, K. R. Mueller, and A. Tkatchenko, Towards exact molecular dynamics simulations with machine-learned force fields. Nature Commun. 9, 3887 (2018).

Navigating chemical space with quantum machine learning

Anatole von Lilienfeld, University of Basel

Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms need to exploit all implicit redundancies present in chemical space. I will discuss recently developed quantum machine learning based approaches for interpolating quantum mechanical observables in compositional and constitutional space. Numerical results from these models indicate controlled accuracy and favourable computational efficiency.

Artificial intelligence methods for discovering novel materials and exotic compounds

Artem R. Oganov, Skolkovo Institute of Science and Technology

Until mid-2000s it was thought that crystal structures are fundamentally unpredictable. This has changed, and a special role in this was played by our evolutionary method/code USPEX (http://uspex-team.org), which now has over 5000 registered users worldwide. This method can be viewed as a type of artificial intelligence, and routinely allows one to predict stable crystal structures for a given chemical composition], and even to predict all stable compounds formed by given elements. I will discuss some of the most important recent results, including:

1. Discovery of novel chemical phenomena at high pressure: transparent non-metallic allotrope of sodium, counterintuitive novel sodium chlorides, chemical reactivity of helium.
2. Prediction of novel surface compounds, with unexpected similarities to high-pressure compounds.
3. Prediction of new high-temperature superconducting polyhydrides, approaching room-temperature superconductivity.
4. Discovery of novel superhard materials, which have the potential for wide industrial application.

I will also mention some applications of another type of artificial intelligence: machine learning methods, including recent prediction of phase diagrams of metals (including both solid-solid transitions and melting).

Effective model estimation for magnetic materials by machine learning

Rio Tamura, University of Tokyo

We developed a method for estimating the effective model of magnetic materials from a given physical quantity by the machine learning based on the Bayesian statistics. In the estimation method, plausible magnetic interactions that explain the given physical quantity are determined by maximizing the posterior distribution. The efficiency of the estimation method was tested by using synthetic magnetization curve data obtained by the classical Heisenberg model. Furthermore, the estimation results of real magnetic materials are shown and speeding up of the effective model estimation by the Bayesian optimization is discussed in this talk.

Spin wave excitations of magnetic metalorganic materials

Johan Hellsvik, Roberto Díaz Pérez, R. Matthias Geilhufe, Martin Månsson, and Alexander V. Balatsky, Nordita, KTH

Materials databases, high throughput computing, and data mining has emerged as powerful tools for screening and rapid prototyping of functional materials. Nordita has taken a step into materials informatics and machine learning with the Organic Materials Database (OMDB) [1] which came online in 2017. The OMDB is an electronic structure database for various organic and organometallic materials, freely accessible via a web interface at https://omdb.mathub.io/. The electronic band structures are calculated using density functional theory that is a standard tool in modern materials science. OMDB's web interface allows users to search for materials with specified target properties using non-trivial queries about their electronic structure, including advanced tools for pattern recognition [2], chemical and physical properties search. The OMDB currently hosts more than 22,000 electronic band structures. For a data set of this size, it is possible to develop and train machine learning models to predict materials properties, thus bypassing the ab initio calculations which are particularly demanding for large chemical unit cells and number of electrons, as is commonly the case for organic materials. Successful training of machine learning models for band gap prediction of organometallic materials has recently been reported in [3]. Materials with competing ground states and phases constitute a challenge for ab initio based modeling. A prominent example are magnetic materials. In a recent paper an important step forward is taken in the development of techniques for predictive modeling of the properties of magnetic solids [4]. The starting point is to consider magnetic materials within the OMDB. Using a ferromagnetic reference spin configuration, the magnetic Hamiltonians are calculated utilizing the infinitesimal rotation technique for calculation of Heisenberg exchange interactions. For these magnetic Hamiltonians quenching simulations down to zero temperature are performed in order to obtain the magnetic ground states. The magnetic excitation spectra are calculated by means of linear spin wave theory and atomistic spin dynamics simulations. The current dataset features collinear as well as noncollinear magnetic materials and has now been released on the OMDB. Representative results and the use of pattern matching algorithms to identify materials with desired properties are highlighted in [4].

[1] S. S. Borysov, R. M. Geilhufe, and A. V. Balatsky, PLOS ONE 12, e0171501 (2017).

[2] S. S. Borysov, B. Olsthoorn, M. B. Gedik, R. M. Geilhufe, and A. V. Balatsky, npj Computational Materials 4, 46 (2018).

[3] B. Olsthoorn, R. M. Geilhufe, S. S. Borysov, and A. V. Balatsky, Advanced Quantum Technologies,1900023 (2019).

[4] J. Hellsvik, R. Díaz Pérez, R. M. Geilhufe, M. Månsson, and A. V. Balatsky, arXiv preprint arXiv:1907.01817 (2019).

New horizons for the fastest, densest and least dissipative brain-inspired computing

Johan H. Mentink, Radboud University

The explosive growth of digital data and its related energy consumption is pushing the need to develop fundamentally new physical principles for faster, smaller and more energy-efficient control of data. Moreover, already today the energy-efficiency of processing technology is limiting their performance. Furthermore, brain-inspired computing schemes offer inherently more energy-efficient computing paradigms for tasks such as pattern recognition. Our research is inspired by the dream to exploit the fastest and most energy-efficient quantum dynamics of magnetic materials to implement the most energy-efficient brain-inspired computing algorithms. As a specific example, we demonstrate experimentally how supervised learning can be achieved using ultrafast optical control of magnetization in technologically relevant Co/Pt thin films at room temperature [1]. Moreover, we present novel theoretical results showing the potential of the recently discovered neural quantum states to simulate the ultrafast dynamics of magnon pairs in Heisenberg antiferromagnets [2]. In addition, we demonstrate that exploring this dynamics inherently opens up the study of so far unexplored physical effects and we show that correlations and therefore entanglement can be coherently manipulated on ultrashort time scales. Finally, we outline the potential of this dynamics for brain-inspired computing at THz frequencies and nanoscale dimensions, suggesting new horizons for brain-inspired computing that are not feasible within further downscaling of existing computing technology platforms.

[1] A. Chakravarty, J.H. Mentink et al., Supervised learning of an opto-magnetic neural network with ultrashort laser pulses. Appl. Phys. Lett. 114, 192407 (2019).

[2] G. Fabiani and J.H. Mentink, Investigating ultrafast quantum magnetism with machine learning. SciPost Physics 7, 004 (2019).

SchNet - an interpretable atomistic neural network

Kristof Schütt, Technical University Berlin

Deep neural networks are emerging as a powerful tool in quantum chemistry and materials science, combining the benefits of electronic structure methods with excellent computational efficiency. Based on the SchNet architecture, we demonstrate that the modular nature of deep models can also be exploited to enhance their versatility and offer insights beyond the basic relations learned by the network. Going beyond the simple prediction of properties, we present the generative model G-SchNet, built on top of SchNet, which may be used to discover novel atomistic systems in equilibrium configuration.

Euclidean Neural Networks* for Emulating Ab Initio Calculations and Generating Atomic Geometries

Tess Smidt, Lawrence Berkeley National Laboratory

Atomic systems (molecules, crystals, proteins, nanoclusters, etc.) are naturally represented by a set of coordinates in 3D space labeled by atom type. This is a challenging representation to use for neural networks because the coordinates are sensitive to 3D rotations and translations and there is no canonical orientation or position for these systems. We present a general neural network architecture that naturally handles 3D geometry and operates on the scalar, vector, and tensor fields that characterize physical systems. Our networks are locally equivariant to 3D rotations and translations at every layer. In this talk, we describe how the network achieves these equivariances and demonstrate the capabilities of our network using simple tasks. We'll also present examples of applying Euclidean networks to multiple applications in quantum chemistry and discuss techniques for using these networks to encode and decode geometry.

* also called Tensor Field Networks and 3D Steerable CNNs

Determining spectrum-structure relation with machine learning techniques

Yi Luo, University of Science and Technology of China and The Royal Institute of Technology (KTH), Stockholm

Spectroscopic techniques have been routinely applied to determine the geometric and electronic structures of complexes in different research fields. However, it is often difficult to extrapolate accurate structural information from the experimental spectra without theoretical simulations. Machine learning offers a powerful tool to significantly increase the efficiency and improve the predictability of the simulations. We have done some exercises recently to use machine learning to predict the structure from vibrational spectrum or vice versa. We have also proposed several useful descriptors to describe the relationship between the protein structure and two-dimensional ultraviolet (2DUV) spectroscopy [1].

[1] S. Ye, W. Hu, X. Li, J. Zhang, K. Zhong, G. Zhang, Y. Luo, S. Mukamel, and J. Jiang, PNAS, 2019, 116, 11612-11617